

# Monte Carlo computation of the Vassiliev knot invariant of degree 2 in the integral representation

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In mathematics there is a wide class of knot invariants that may be expressed in the form of multiple line integrals computed along the trajectory  $C$  describing the spatial conformation of the knot. In this work it is addressed the problem of evaluating invariants of this kind in the case in which the knot is discrete, i. e. its trajectory is constructed by joining together a set of segments of constant length. Such discrete knots appear almost everywhere in numerical simulations of systems containing one dimensional ring-shaped objects. Examples are polymers, the vortex lines in fluids and superfluids like helium and other quantum liquids. Formally, the trajectory of a discrete knot is a piecewise smooth curve characterized by sharp corners at the joints between contiguous segments. The presence of these corners spoils the topological invariance of the knot invariants considered here and prevents the correct evaluation of their values. To solve this problem, a smoothing procedure is presented, which eliminates the sharp corners and transforms the original path  $C$  into a curve that is everywhere differentiable. The procedure is quite general and can be applied to any discrete knot defined off or on lattice. This smoothing algorithm is applied to the computation of the Vassiliev knot invariant of degree 2 denoted here with the symbol  $\varrho(C)$ . This is the simplest knot invariant that admits a definition in terms of multiple line integrals. For a fast derivation of  $\varrho(C)$ , it is used a Monte Carlo integration technique. It is shown that, after the smoothing, the values of  $\varrho(C)$  may be evaluated with an arbitrary precision. Several algorithms for the fast computation of the Vassiliev knot invariant of degree 2 are provided.

## I. INTRODUCTION

There are many situations in which it is necessary to distinguish the topological properties of ring-shaped quasi one-dimensional objects. This is for instance the case of polymers<sup>1,2</sup>, vortex structures in nematic liquid crystals<sup>3</sup>,  $^3\text{He}$  superfluid<sup>4</sup> and disclination lines in chiral nematic colloids<sup>5</sup>. In order to ascertain the type of a knot, it is possible to apply the so-called knot invariants. These mathematical quantities, which remain unchanged under ambient isotopy, are usually represented in the form of polynomials, like for example the Alexander<sup>6</sup> or the HOMFLY polynomials<sup>7</sup>. Alternatively, certain knot invariants may be defined in terms of multiple curvilinear integrals, in which the integrations are performed along the spatial trajectory of the knot or elements of it<sup>8-10</sup>. Particularly important for applications is the case in which knots are constructed by joining together at their ends a set of  $N$  segments. Discrete knots of this kind are in fact the most common concrete realizations of knots in numerical simulations. Formally, a discrete knot is  $C^0$ -curve which is piecewise smooth and is characterized by sharp corners at the joints between contiguous segments. While there exist already well established mathematical algorithms in order to compute numerically polynomial knot invariants, see for instance the pioneering work<sup>11</sup>, there are not many studies concerning the numerical computation of knot invariants given in the form of multiple line integrals for such discrete knots. Of course, the calculation of line integrals over discrete data is a textbook subject<sup>12,13</sup>. Moreover, problems in which knots are discretized using splines, have been investigated for example in<sup>14</sup>. However, we are faced with a somewhat different problem, which arises due to the fact that knot invariants expressed as multiple curvilinear integrals are not well defined in the case of discrete knots. The reason of this failure is related to the presence of the non-smooth corners at the joints between two contiguous segments. As a consequence, the main goal pursued here is to replace the piecewise smooth curves representing a discrete knot with more regular ones. To obtain a smoothing algorithm that is able to perform this replacement for general discrete knots without destroying their topology, a strategy has been adopted that can be briefly summarized as follows. First, the sharp corners are surrounded with spheres whose radii are chosen in such a way that they do not intersect with themselves and with other elements of the knot. After that, the elements containing the corners inside the spheres are substituted with arcs of smooth curves. This procedure transforms the original trajectories into  $G^1$ -curves<sup>29</sup> without altering their

topological configurations. As an application, the case of the Vassiliev knot invariant of degree  $2^{16}$  of a knot  $C$ , denoted here  $\varrho(C)$ , is worked out. The main advantages of choosing this invariant are its relative simplicity and the fact that its exact values for different knots can be computed analytically. In this way, it is possible to perform a comparison between numerical and analytical results. After the smoothing procedure proposed in this work, it becomes possible to calculate  $\varrho(C)$  numerically with an arbitrarily high precision.

Despite its simplicity, the Vassiliev invariant of degree 2 requires the evaluation of complicated quadruple and triple line integrals. Having in mind concrete applications, in which the knot invariant  $\varrho(C)$  must be computed millions of times, see for instance Ref.<sup>17</sup>, we have proposed here several strategies to accelerate its calculation. It turns out that Monte Carlo integration algorithms are faster than traditional integration methods<sup>18</sup>. For this reason, a Monte Carlo integration scheme is adopted and explained in details. Moreover, several tricks to speed up the computation of  $\varrho(C)$ , that are specific to particular applications or situations, are presented. Since the time for evaluating  $\varrho(C)$  is sensitive to the number of segments  $N$  composing the knot, but not on its length, we have provided an algorithm to reduce by a factor three the number of segments without changing the topology of the knot. This algorithm is valid for knots defined on a simple cubic lattice. Secondly, it is shown that the number of points of the trajectory  $C$  to be sampled during the Monte Carlo integration procedure may be considerably decreased when the knot invariant  $\varrho(C)$  is used in order to detect topology changes that may potentially occur after a random transformation of an element of the trajectory of the knot. Such random transformations, like for instance the pivot moves<sup>19</sup>, the pull moves<sup>20</sup> and the BFACF moves<sup>21</sup>, are extensively exploited in numerical simulations of polymer knots.

The material presented in this paper is divided as follows. In the next Section, the Vassiliev invariant of degree 2 is defined in the case of general smooth curves. In Section III we specialize to general discrete knots, which are represented as piecewise smooth curves parametrized by a continuous variable  $S \in [0, N]$ . In this way, the calculation of  $\varrho(C)$  is reduced to that of multiple integrals over a set of variables  $S, T, U, V \in [0, N]$  and can be tackled by standard Monte Carlo techniques. A numerical version of the so-called framing<sup>22</sup> procedure is implemented in order to regularize singularities that are possibly arising in some of the terms to be integrated. While it is analytically proven that the sum of all these terms is always finite, the presence of singularities in single terms may spoil the result of

the numerical integration. A smoothing procedure is presented in Section IV in order to transform a general discrete knot into a  $G^1$ -curve. This procedure allows the calculation of  $\varrho(C)$  by Monte Carlo integration techniques with an arbitrary precision depending on the number of used samples. In Section V a few methods to speed up the calculations are discussed. Finally, the conclusions are drawn in Section VI.

## II. THE VASSILIEV INVARIANT OF DEGREE 2

Let us consider a general knot of length  $L$  in the flat three dimensional space  $\mathbb{R}^3$  spanned by a set of cartesian coordinates  $\mathbf{x} = (x^1, x^2, x^3)$ . The space indexes are labeled with greek letters  $\mu, \nu, \rho, \dots = 1, 2, 3$ . The Alexander-Briggs notation for denoting knots is used. In this Section, the spatial trajectory  $C$  formed in the space by the knot is chosen to be a smooth curve  $\mathbf{x}(s) : [0, L] \rightarrow \mathbb{R}^3$  parametrized using its arc-length  $0 \leq s \leq L$ . Different points on the curve corresponding to different values of the arc-length  $s, t, u$  and  $v$  will be denoted with the symbols  $x^\mu(s), y^\nu(t), z^\rho(u)$  and  $w^\sigma(v)$ , with  $\mu, \nu, \rho, \sigma = 1, 2, 3$ . As a convention, summation over repeated indexes is understood. Moreover, let  $\dot{x}^\mu(s)$  be the derivative of  $x^\mu(s)$  with respect to  $s$ . An analogous notation holds for  $\dot{y}^\nu(t), \dot{z}^\rho(u)$  and  $\dot{w}^\sigma(v)$ . Finally,  $\epsilon_{\mu\nu\rho}$  is the completely antisymmetric tensor uniquely defined by the condition  $\epsilon_{123} = 1$ .

With the above settings, the Vassiliev knot invariant of degree 2  $\varrho(C)$  of a knot  $C$  can be written as follows<sup>9,10,23</sup>:

$$\varrho(C) = \varrho_1(C) + \varrho_2(C) \quad (1)$$

where  $\varrho_1(C)$  and  $\varrho_2(C)$  are two path ordered multiple line integrals given by:

$$\varrho_1(C) = \int_0^L ds \int_0^s dt \int_0^t du F_1(\mathbf{x}(s), \mathbf{y}(t), \mathbf{z}(u); \dot{\mathbf{x}}(s), \dot{\mathbf{y}}(t), \dot{\mathbf{z}}(u)) \quad (2)$$

and

$$\varrho_2(C) = \int_0^L ds \int_0^s dt \int_0^t du \int_0^u dv F_2(\mathbf{x}(s), \mathbf{y}(t), \mathbf{z}(u), \mathbf{w}(v); \dot{\mathbf{x}}(s), \dot{\mathbf{y}}(t), \dot{\mathbf{z}}(u), \dot{\mathbf{w}}(v)) \quad (3)$$

The quantities  $F_1$  and  $F_2$  are defined below:

$$\begin{aligned}
-32\pi^3 F_1(\mathbf{x}, \mathbf{y}, \mathbf{z}; \dot{\mathbf{x}}, \dot{\mathbf{y}}, \dot{\mathbf{z}}) = & C_1 C_2 C_3 [\dot{\mathbf{y}} \cdot \dot{\mathbf{z}}(\dot{\mathbf{x}} \cdot \mathbf{c}) + \dot{\mathbf{x}} \cdot \dot{\mathbf{z}}(\dot{\mathbf{y}} \cdot \mathbf{b}) + \dot{\mathbf{x}} \cdot \dot{\mathbf{y}}(\dot{\mathbf{z}} \cdot \mathbf{a})] \\
& - C_1 C_2^2 C_3 \left[ \dot{\mathbf{y}} \cdot (\mathbf{a} \times \mathbf{b}) \left( \mathbf{a} + \mathbf{b} \frac{a}{b} \right) \cdot (\dot{\mathbf{z}} \times \dot{\mathbf{x}}) \right. \\
& \left. + \dot{\mathbf{z}} \cdot (\mathbf{a} \times \mathbf{b}) \left( \mathbf{b} + \mathbf{a} \frac{b}{a} \right) \cdot (\dot{\mathbf{y}} \times \dot{\mathbf{x}}) \right] \\
& + C_1 C_2 \left[ \dot{\mathbf{y}} \cdot (\mathbf{a} \times \mathbf{b}) \left( \mathbf{b} \frac{c-a}{b^2} + \mathbf{c} \frac{a+b}{c^2} \right) \cdot (\dot{\mathbf{z}} \times \dot{\mathbf{x}}) \right. \\
& \left. + \dot{\mathbf{z}} \cdot (\mathbf{a} \times \mathbf{b}) \left( \mathbf{a} \frac{c-b}{a^2} - \mathbf{c} \frac{a+b}{c^2} \right) \cdot (\dot{\mathbf{y}} \times \dot{\mathbf{x}}) \right] \quad (4)
\end{aligned}$$

$$F_2(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w}; \dot{\mathbf{x}}, \dot{\mathbf{y}}, \dot{\mathbf{z}}, \dot{\mathbf{w}}) = \frac{1}{8\pi^2} \left( \dot{\mathbf{x}} \cdot \left( \dot{\mathbf{z}} \times \frac{\mathbf{b}}{b^3} \right) \right) \left( \dot{\mathbf{y}} \cdot \left( \dot{\mathbf{w}} \times \frac{\mathbf{c}}{c^3} \right) \right) \quad (5)$$

In Eqs. (4) and (5) we have put:

$$\mathbf{a} = \mathbf{y} - \mathbf{x} \quad \mathbf{b} = \mathbf{z} - \mathbf{x} \quad \mathbf{c} = \mathbf{y} - \mathbf{z} \quad (6)$$

and

$$C_1 = \frac{2\pi}{abc} \quad (7)$$

$$C_2 = \frac{1}{ab + a_\mu b_\mu} \quad (8)$$

$$C_3 = a + b - c \quad (9)$$

Let us note that in Eq. (8) we have used a convention for which repeated indexes are summed. It is known that the above defined  $\varrho(C)$  is related to the second coefficient  $a_2(C)$  of the Conway polynomial of a knot  $C$  through the following relation<sup>10</sup>:

$$a_2(C) = \frac{1}{2} \left[ \varrho(C) + \frac{1}{12} \right] \quad (10)$$

The coefficients of the Conway polynomials can be computed analytically for every knot topology.  $\varrho(C)$  is the simplest knot invariant expressed in the form of contour integrals. It is also called the Casson knot invariant, see Ref.<sup>24</sup>

### III. THE VASSILIEV KNOT INVARIANT OF DEGREE 2 FOR DISCRETE KNOTS

In principle, analytical computations of  $\varrho(C)$  are possible if the curve  $\mathbf{x}(s)$  describing the knot  $C$  is given in parametric form. However, a close expression of  $\mathbf{x}(s)$  for a knot of

arbitrary shape usually does not exist and one should pass to a discrete representation of it. To switch from continuous functions to discrete ones is one of the most standard problems of numerical integration. In the present case, the situation is opposite. For instance, in numerical simulations involving ring-shaped objects with nontrivial topological configurations the knots are already discrete by construction. The real difficulty is rather that knot invariants expressed in the form of multiple line integrals like  $\varrho(C)$ , cease to be topological invariants if knots are discrete. In order to restore this invariance, a procedure that is able to smooth up a discrete knot transforming it from a  $C^0$ –curve into a  $G^1$ –curve without destroying its topological configuration is needed. Such a procedure will be presented in the following.

First of all, to be concrete, let us define the discrete knot as a set of  $N$  points:

$$\mathbf{x}_i = \mathbf{x}(s_i) \quad \begin{cases} i = 1, \dots, N \\ 0 < s_1 < s_2 < \dots < s_N = L \end{cases} \quad (11)$$

joined together by  $N$  segments

$$\mathbf{l}_i = \mathbf{x}_i - \mathbf{x}_{i-1} \quad i = 2, \dots, N \quad (12)$$

$$\mathbf{l}_1 = \mathbf{x}_1 - \mathbf{x}_N \quad (13)$$

The discrete knot may be regarded as a piecewise smooth curve  $\mathbf{X}(S) : [0, N] \rightarrow \mathbb{R}$ , where

$$0 \leq S \leq N \quad (14)$$

Explicitly, a general point located on the  $i$ –th segment of  $\mathbf{X}(S)$  is identified by the relations:

$$\mathbf{X}(S) = \mathbf{x}_{i-1} + (S - [S])\mathbf{l}_i \quad \begin{cases} i - 1 < S \leq i \\ i = 2, \dots, N \end{cases} \quad (15)$$

and

$$\mathbf{X}(S) = \mathbf{x}_N + (S - [S])\mathbf{l}_1 \quad 0 < S \leq 1 \quad (16)$$

In the above equations  $[S]$  denotes the integer part of  $S$ . The example of a curve  $\mathbf{X}(S)$  with eight segments is given in Fig. 1. In the limit in which  $N$  approaches infinity and the lengths of the  $N$  segments become vanishingly small, a continuous representation of the knot is obtained. If  $l_i = |\mathbf{l}_i|$  denotes the length of the  $i$ –th segment and  $\Lambda_N = \sum_{i=1}^N l_i$  is the total length of the discretized curve, then the length  $L$  of the continuous knot is given by:

$$\lim_{\substack{N \rightarrow \infty \\ l_i \rightarrow 0, i=1, \dots, N}} \Lambda_N = L \quad (17)$$

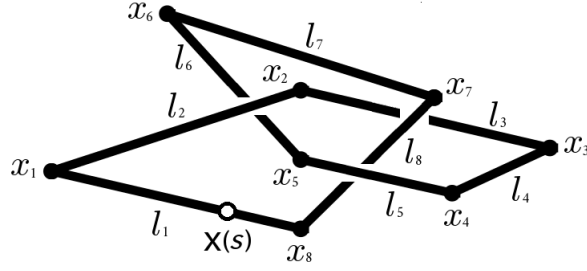


FIG. 1. Example of an off lattice discrete knot (a trefoil) with only eight sides. A generic point  $\mathbf{X}(S)$  on the trajectory is shown.

At this point it is possible to compute the contributions  $\varrho_1(C)$  and  $\varrho_2(C)$  to the Vassiliev invariant of degree 2 for a general discrete knot  $C$  with trajectory  $\mathbf{X}(S)$ . With the above definitions, the same prescriptions of Eqs. (2) and (3), which are valid for a smooth curve  $\mathbf{x}(s)$ , can be formally applied. It is sufficient to substitute the smooth trajectories  $\mathbf{x}(s)$ ,  $\mathbf{y}(t)$ ,  $\mathbf{z}(u)$  and  $\mathbf{w}(v)$  with their discrete analogs  $\mathbf{X}(S)$ ,  $\mathbf{Y}(T)$ ,  $\mathbf{Z}(U)$  and  $\mathbf{W}(V)$ . In the following, the symbols  $F_1(S, T, U)$  and  $F_2(S, T, U, V)$  will denote the integrands of Eqs. (2) and (3) in the case of a discrete knot in which the variables  $s, t, u, v$  are replaced by  $S, T, U, V$ . Of course, in these equations the upper integration boundary  $L$  should be replaced by  $N$ . The derivatives  $\dot{\mathbf{X}}(S)$ ,  $\dot{\mathbf{Y}}(T)$ ,  $\dot{\mathbf{Z}}(U)$  and  $\dot{\mathbf{W}}(V)$  require some more care. On the  $i$ -th segment, away from the joints, the curve is trivially smooth and the computation of  $\dot{\mathbf{X}}(S)$ ,  $\dot{\mathbf{Y}}(T)$ ,  $\dot{\mathbf{Z}}(U)$ ,  $\dot{\mathbf{W}}(V)$  is straightforward:

$$\dot{\mathbf{X}}(S) = \mathbf{l}_i \quad \begin{cases} i-1 < S < i \\ i = 2, \dots, N \end{cases} \quad (18)$$

$$\dot{\mathbf{X}}(S) = \mathbf{l}_1 \quad 0 < S < 1 \quad (19)$$

At the points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  in which the segments join together, instead, the curve  $\mathbf{X}(S)$  ceases to be differentiable. Still, it is possible to define formally the derivatives at these points by assuming that the tangent to the discrete trajectory in  $\mathbf{x}_{i-1}$  is proportional to the segment  $\mathbf{l}_i$ . Using this convention we obtain:

$$\dot{\mathbf{X}}(i-1) = \mathbf{l}_i \quad i = 2, \dots, N \quad (20)$$

$$\dot{\mathbf{X}}(N) = \mathbf{l}_1 \quad (21)$$

The above definition is clearly not unique. Analogously, we could have chosen  $\dot{\mathbf{X}}(i-1) = \mathbf{l}_{i-1}$ ,  $i = 2, \dots, N$  and  $\dot{\mathbf{X}}(N) = \mathbf{l}_N$ .

With the prescriptions (14–16) and (18–21) given above in order to parametrize the discrete knot, the evaluation of the two multiple line integrals appearing in Eqs. (2) and (3) may be performed using numerical integration techniques like the rectangle rule method, trapezoidal rule method, Simpson’s rule method, Newton-Cotes method, Romberg method, Gauss method etc.<sup>25</sup> Let us note that the variables  $S, T$  and  $U$  appearing in  $\varrho_1(C)$ , see Eq. (2), span a space of volume

$$V_1 = \frac{N^3}{6} \quad (22)$$

while the variables  $S, T, U$  and  $V$  appearing in Eq. (3) span a space of volume

$$V_2 = \frac{N^4}{24} \quad (23)$$

When  $N$  is large, these volumes become too large to be treated with quadrature methods and it is more convenient to compute the right hand sides of Eqs. (2) and (3) using a Monte Carlo approach<sup>30</sup>. For the integral of a function of  $m$  variables  $f(\xi_1, \dots, \xi_m)$  with integration boundaries like those in Eqs. (2) and (3), it can be applied to this purpose the general formula:

$$\begin{aligned} & \int_{a_1}^{b_1} d\xi_1 \int_{a_2}^{\xi_1} d\xi_2 \cdots \int_{a_m}^{\xi_{m-1}} d\xi_m f(\xi_1, \dots, \xi_m) \\ & \approx \frac{1}{n} \left[ \sum_{i=1}^n f(\xi_1^{(i)}, \dots, \xi_m^{(i)}) (b_1 - a_1) \prod_{\sigma=2}^m (\xi_\sigma^{(i)} - a_\sigma) \right] \end{aligned} \quad (24)$$

where the  $\xi_\sigma^{(i)}$ ’s,  $i = 1, \dots, n$  and  $\sigma = 1, \dots, m$  denote randomly chosen variables in the range:

$$\begin{aligned} & [a_1, b_1] \quad \text{when } \sigma = 1 \\ & [a_\sigma, \xi_\sigma] \quad \text{when } \sigma = 2, \dots, m \end{aligned} \quad (25)$$

The naive procedure discussed above is plagued by two systematic errors. First of all, the discrete knots treated here so far are not smooth at the joints between two segments. On a simple cubic lattice, it is possible to verify that the values of  $\varrho(C)$  computed for a discrete knot are always greater than the analytical values, a fact that is certainly related to the presence of sharp corners at these joints. This excess from the exact value is roughly proportional to the number of the corners. The second source of errors is connected with possible singularities arising in the integrands  $F_1(S, T, U)$  and  $F_2(S, T, U, V)$  appearing in



Eqs. (2) and (3). Of course, globally both  $F_1(S, T, U)$  and  $F_2(S, T, U, V)$  are regular for every value of  $S, T, U$  and  $V$  as it has been proved in<sup>10</sup>. However, the fact that  $F_1(S, T, U)$  and  $F_2(S, T, U, V)$  are finite everywhere does not prevent the presence of singularities in single terms entering in the expressions of these integrands. Looking at Eqs. (4–9), it is easy to realize that some of these terms diverge whenever one or more of the following conditions are met:

$$\mathbf{Y}(T) - \mathbf{X}(S) = 0 \quad (26)$$

$$\mathbf{Z}(U) - \mathbf{X}(S) = 0 \quad (27)$$

$$\mathbf{Y}(T) - \mathbf{Z}(U) = 0 \quad (28)$$

$$|\mathbf{Y}(T) - \mathbf{X}(S)| |\mathbf{Z}(U) - \mathbf{X}(S)| + (\mathbf{Y}(T) - \mathbf{X}(S)) \cdot (\mathbf{Z}(U) - \mathbf{X}(S)) = 0 \quad (29)$$

When summed together, these singularities disappear making  $F_1(S, T, U)$  and  $F_2(S, T, U, V)$  finite, but for the purposes of numerical calculations a regularization is needed to remove them. To this purpose, a suitable regularization is the framing of the trajectories described in<sup>22</sup>. In the present context, the framing consists in a slight deformation of the curves  $\mathbf{X}(S)$ ,  $\mathbf{Y}(T)$ ,  $\mathbf{Z}(U)$  and  $\mathbf{W}(V)$  of the kind:

$$X^\mu(S) \longrightarrow X_{\epsilon_X}^\mu(S) = X^\mu(S) + \epsilon n^\mu(S) \quad (30)$$

$$Y^\nu(T) \longrightarrow Y_{\epsilon_Y}^\nu(T) = Y^\nu(T) + 2\epsilon n^\nu(T) \quad (31)$$

$$Z^\rho(U) \longrightarrow Z_{\epsilon_Z}^\rho(U) = Z^\rho(U) + 3\epsilon n^\rho(U) \quad (32)$$

$$W^\sigma(V) \longrightarrow W_{\epsilon_W}^\sigma(V) = W^\sigma(V) + 4\epsilon n^\sigma(V) \quad (33)$$

where  $n^\mu(S)$ ,  $n^\nu(T)$ ,  $n^\rho(U)$  and  $n^\sigma(V)$  denote unit vectors normal to the trajectories  $\mathbf{X}(S)$ ,  $\mathbf{Y}(T)$ ,  $\mathbf{Z}(U)$  and  $\mathbf{W}(V)$  respectively.  $\epsilon$  is a very small parameter. Clearly, the prescription provided in Eqs. (30–33) is able to remove the divergences at the locations defined in (26–29). Moreover, in the limit  $\epsilon \rightarrow 0$  one recovers the exact expression of  $\varrho(C)$  independently of the choice of the normal unit vectors  $n^\mu(S)$ ,  $n^\nu(T)$ ,  $n^\rho(U)$  and  $n^\sigma(V)$  as it has been proved in Ref.<sup>10</sup>. For example, in calculations on a simple cubic lattice the framing can be implemented by small shifts of the trajectories  $\mathbf{X}(S)$ ,  $\mathbf{Y}(T)$ ,  $\mathbf{Z}(U)$  and  $\mathbf{W}(V)$  along the direction  $(1, 1, 1)$ . This is sufficient to regularize all potentially divergent terms in  $F_1(S, T, U)$  and  $F_2(S, T, U, V)$  without creating dangerous intersections of the trajectories of the shifted knots that are forbidden. From our simulations it turns out that the results of the computations of  $\varrho(C)$  are not much sensitive to the values of the  $\epsilon$ -parameter. This is connected to the fact that

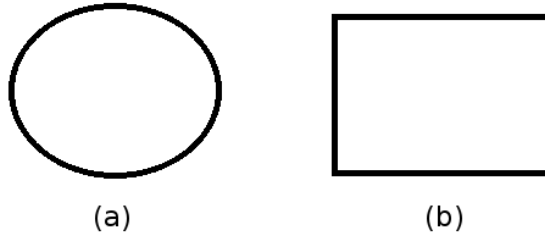


FIG. 2. (a) An unknot with smooth trajectory; (b) An unknot defined on a simple cubic lattice.

the points in which the singularity conditions of Eqs. (26–29) are satisfied represent a very small subset of the set of all sampled points.

To eliminate the systematic error due to the presence of the sharp corners is much more difficult. This will be the subject of the next Section, in which a smoothing procedure will be presented, that transforms the curve  $\mathbf{X}(S)$  into a curve whose first derivatives exist and are continuous.

#### IV. MONTE CARLO EVALUATION OF $\varrho(C)$ WITH SMOOTHING PROCEDURE OF DISCRETE KNOTS

The effect of the sharp corners at the joints of the segments on the computation of  $\varrho(C)$  can be checked using the very simple example of an unknot with two different trajectories:

- A smooth circle defined by the parametric curve  $x^1(\theta) = \cos(\theta)$ ,  $x^2(\theta) = \sin(\theta)$  and  $x^3(\theta) = 0$ ,  $\theta \in [0, 2\pi]$ , see Fig. 2(a).
- A square defined on a simple cubic lattice as shown in Fig. 2(b).

The exact value of the Vassiliev invariant of degree 2 for the unknot is  $-\frac{1}{12} \sim -0.083$ . The Monte Carlo computation of  $\varrho(C)$  gives a result that is very near to the exact one in the case of the circle:  $\varrho(C) = -0.083 \pm 1.72 \times 10^{-4}$ . However, for the square we obtain  $\varrho(C) = 0.050 \pm 1.17 \times 10^{-4}$ , which is far from the expected result. To avoid these ambiguities in the calculation of  $\varrho(C)$  for discrete knots, a smoothing procedure for eliminating the sharp corners will be presented.

The idea is to replace at each of the joints  $\mathbf{x}_i$  the neighborhoods of the corners with smooth arcs of curves whose ends are glued together in such a way that the whole knot will

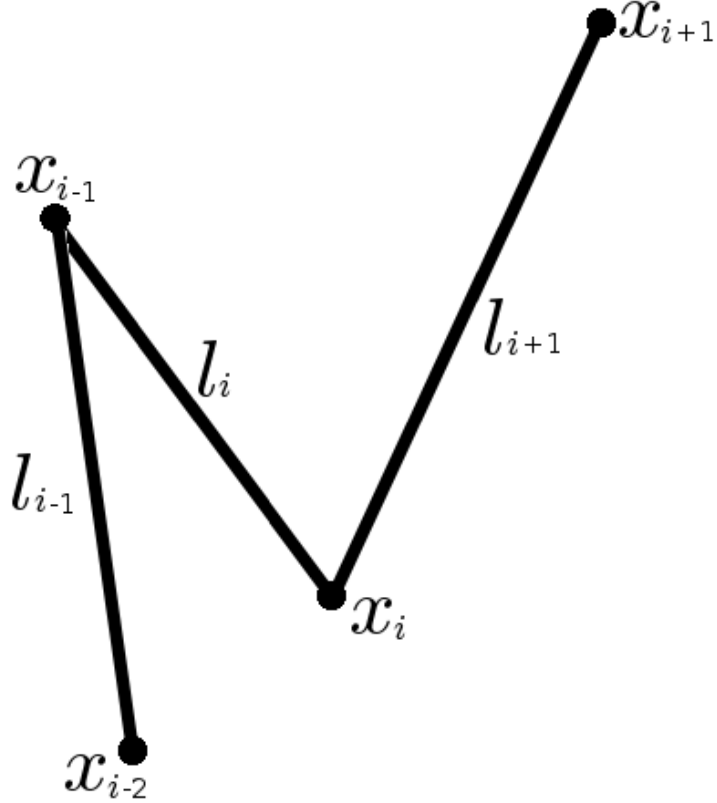


FIG. 3. This figure shows the three contiguous segments  $l_{i-1}$ ,  $l_i$  and  $l_{i+1}$  subtending the corners  $x_{i-1}$  and  $x_i$ .

be a continuous curve with its first derivative. To illustrate the method, we pick up a triplet of contiguous segments  $l_{i-1}$ ,  $l_i$  and  $l_{i+1}$ , see Fig. 3. It is easy to realize that the segment  $l_i$  is shared by the two corners centered at the points  $x_{i-1}$  and  $x_i$ . This is not desirable for our purposes. To achieve the goal that each corner will be subtended by couples of segments that are not in common with those related to other corners, we divide each segment  $l_i$ ,  $i = 1, \dots, N$ , into the three subsegments:

$$l_i^- = x_i^- - x_{i-1} \quad (34)$$

$$l_i^0 = x_i^+ - x_i^- \quad (35)$$

$$l_i^+ = x_i^+ - x_i \quad (36)$$

The ends  $\mathbf{x}_i^-$  and  $\mathbf{x}_i^+$  are fixed in such a way that the lengths of  $\mathbf{l}_i^-, \mathbf{l}_i^0$  and  $\mathbf{l}_i^+$  are  $d'_{i-1}$ ,  $l_i - d'_{i-1} - d_i$  and  $d_i$  respectively (see Fig. 4):

$$\mathbf{x}_i^- = \mathbf{x}_{i-1} + \frac{\mathbf{x}_i - \mathbf{x}_{i-1}}{l_i} d'_{i-1} \quad (37)$$

$$\mathbf{x}_i^+ = \mathbf{x}_i + \frac{\mathbf{x}_{i-1} - \mathbf{x}_i}{l_i} d_i \quad (38)$$

The values of  $d'_{i-1}$  and  $d_i$  will be chosen in such a way that

- 1) the topology of the discrete knot is not destroyed after the smoothing procedure and
- 2) the length of none of the subsegments  $\mathbf{l}_i^\pm$  and  $\mathbf{l}_i^0$  exceeds  $\frac{l_i}{2}$ .

An algorithm to determine  $d'_{i-1}$  and  $d_i$  will be provided later. After performing the above splitting for  $\mathbf{l}_{i-1}$ ,  $\mathbf{l}_i$  and  $\mathbf{l}_{i+1}$ , the subsegments  $\mathbf{l}_{i-1}^+$  and  $\mathbf{l}_i^-$  subtend the corner centered in  $\mathbf{x}_{i-1}$ , while the corner in  $\mathbf{x}_i$  is subtended by  $\mathbf{l}_i^+$  and  $\mathbf{l}_{i+1}^-$ . Thus, if all segments composing the knot are splitted in this way, we arrive at the desired situation in which none of the segments subtending a given corner is shared by another corner. At this point, each corner subtended by the couples of segments  $\mathbf{l}_i^+, \mathbf{l}_{i+1}^-$  for  $i = 1, \dots, N-1$  and  $\mathbf{l}_N^+, \mathbf{l}_1^-$  for  $i = N$  may be substituted by arcs of smooth curves as shown in Fig. 5.

As an arc of a smooth curve replacing the generic corner in  $\mathbf{x}_i$  subtended by the subsegments  $\mathbf{l}_i^+$  and  $\mathbf{l}_{i+1}^-$ , it is possible to use the ansatz (the superscript  $+$  refers to  $\mathbf{l}_i^+$ , while the superscript  $-$  refers to  $\mathbf{l}_{i+1}^-$ ):

$$\mathbf{X}_i^+(S) = -\frac{d_i}{l_i} \frac{l_{i+1}}{d'_i} \frac{\sin \theta_i^+(S)}{1 - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \frac{d_i}{l_i} \frac{l_{i+1}}{d'_i}} \mathbf{l}_i^+ - \frac{(\cos \theta_i^+(S) - 1)}{1 - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \frac{l_i}{d_i} \frac{d'_i}{l_{i+1}}} \mathbf{l}_{i+1}^- + \mathbf{l}_i^+ + \mathbf{x}_i \quad (39)$$

$$\mathbf{X}_{i+1}^-(S) = -\frac{(\sin \theta_{i+1}^-(S) - 1)}{1 - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \frac{d_i}{l_i} \frac{l_{i+1}}{d'_i}} \mathbf{l}_i^+ - \frac{l_i}{d_i} \frac{d'_i}{l_{i+1}} \frac{\cos \theta_{i+1}^-(S)}{1 - \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \frac{l_i}{d_i} \frac{d'_i}{l_{i+1}}} \mathbf{l}_{i+1}^- + \mathbf{l}_{i+1}^- + \mathbf{x}_i \quad (40)$$

with

$$\theta_i^+(S) = \left( \frac{l_i}{2d_i} (S - [S]) - \frac{l_i - d_i}{2d_i} \right) \frac{\pi}{2} \quad \frac{l_i - d_i}{l_i} \leq S - [S] \leq 1 \quad (41)$$

$$\theta_{i+1}^-(S) = \left( \frac{l_{i+1}}{2d'_i} (S - [S]) + \frac{1}{2} \right) \frac{\pi}{2} \quad 0 \leq S - [S] \leq \frac{d'_i}{l_{i+1}} \quad (42)$$

Eqs. (39–42) are defined for  $i = 1, \dots, N-1$ . Their extension to the corner in  $\mathbf{x}_N$  is straightforward. It is easy to verify that after replacing the sharp corners at the vertices  $\mathbf{x}_i$  with the arcs of curve  $\mathbf{X}_i^+(S)$  and  $\mathbf{X}_{i+1}^-(S)$  a  $G^1$ -curve is obtained:

1. First of all, at the point connecting  $\mathbf{X}_i^+(S)$  and  $\mathbf{X}_{i+1}^-(S)$ , occurring when  $\theta_i^+(1) = \theta_{i+1}^-(0) = \frac{\pi}{4}$ , it is possible to verify that the curve obtained after the replacement is continuous.

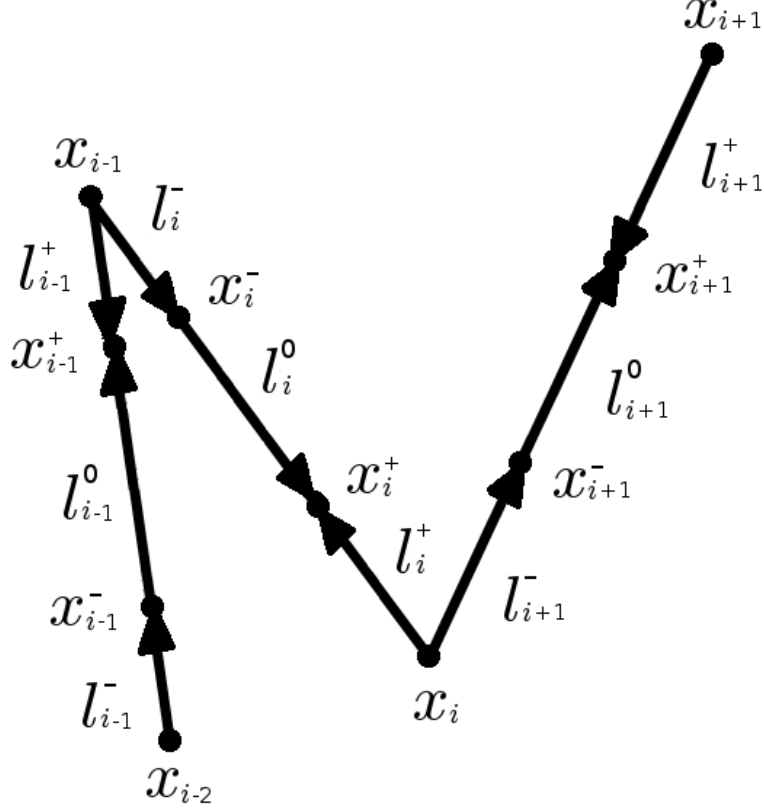


FIG. 4. The segments  $l_{i-1}$ ,  $l_i$  and  $l_{i+1}$  of Fig. 3 are split into three subsegments in such a way that the corners in  $x_{i-1}$  and  $x_i$  are subtended by segments that are not in common. In the given example, after the splitting, the corner in  $x_{i-1}$  is subtended by the subsegments  $l_{i-1}^+$  and  $l_i^-$ . The corner in  $x_i$  is subtended instead by  $l_i^+$  and  $l_{i+1}^-$ .

2. Second, both  $\mathbf{X}_i^+(S)$  and  $\mathbf{X}_{i+1}^-(S)$  are differentiable and their derivatives, which are continuous, do coincide.
3. Third, the unit tangent vectors computed on the subsegments  $l_i^0$  coincide with the unit tangent vectors computed in the subsegments  $l_i^+$  at the point  $x_i^+$  in which these subsegments are connected together. The same is true in the case of the point  $x_i^-$  in which  $l_i^-$  and  $l_i^0$  are joined. To show that, we note that  $\mathbf{X}_i^+(S)$  maps the subsegment  $l_i^+$  into a continuous arc of a curve with unit tangent vector  $\mathbf{t}_i^+$  at the end point  $x_i^+$  given by  $\mathbf{t}_i^+ = -\frac{l_i^+}{l_i^+}$ . To have a  $G^1$ -curve,  $\mathbf{t}_i^+$  must coincide with the tangent  $\mathbf{t}_i^0$  computed at  $x_i^+$ , but staying on the subsegment  $l_i^0$ . It is easy to check using the parametrization

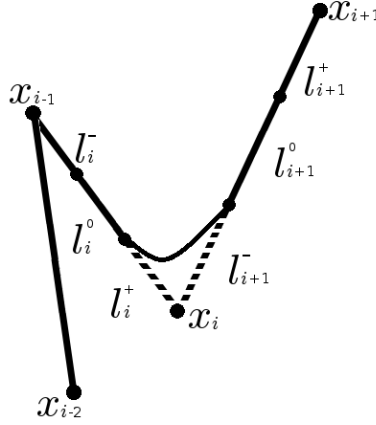


FIG. 5. Substitution of the sharp corner in  $x_i$  by an arc of the smooth curve defined in Eqs. (39–40). It is shown that the subsegments  $l_i^+$  and  $l_{i+1}^-$  subtending this corner are replaced by a smooth trajectory. The replaced part has been denoted with dashed lines.

(15–16) of the knot on  $l_i^0$  that  $t_i^0 = \frac{l_i}{l_i}$ . Thus, taking into account the fact that  $l_i^+$  and  $l_i$  are antiparallel, it is possible to conclude that  $t_i^+ = t_i^0$  as desired. As well, the unit tangent vector computed on the curve  $\mathbf{X}_{i+1}^-(S)$  at  $x_{i+1}^-$  coincides with the unit tangent vector computed on  $l_{i+1}^0$  at the point  $x_{i+1}^-$ .

4. Finally, even if this is not necessary for the present purpose, we have also checked numerically that, for a wide range of the variable  $x = \frac{d_i l_{i+1}}{d_{i+1} l_i}$  entering the expressions of  $\mathbf{X}_i^+(S)$  and  $\mathbf{X}_{i+1}^-(S)$ , more precisely for  $0.01 \leq x \leq 100$ , the distance between the point  $x_i$  and any of the points of the curve  $\mathbf{X}_i^+(S)$  ( $\mathbf{X}_{i+1}^-(S)$ ) never grows beyond a fraction of  $d_i$  ( $d_i'$ ).

Now we know that the knot obtained after substituting the sharp corners with smooth arcs of curves is a  $G^1$ –curve. However, we have to verify that the topology of the smoothed knot and that of the original discrete one are the same. In particular, we have to be sure that, after the replacement of a corner with an arc of a smooth curve, the dangerous situation depicted in Fig. 6 does not occur. This goal will be achieved by a careful definition of the lengths of the segments  $l_i^\pm$  and  $l_i^0$ . To this purpose, we have to derive suitable values  $d_i, d_i'$  for  $i = 1, \dots, N$ . The case  $i = N$  is quite an exception, because the segment  $l_N$  is followed

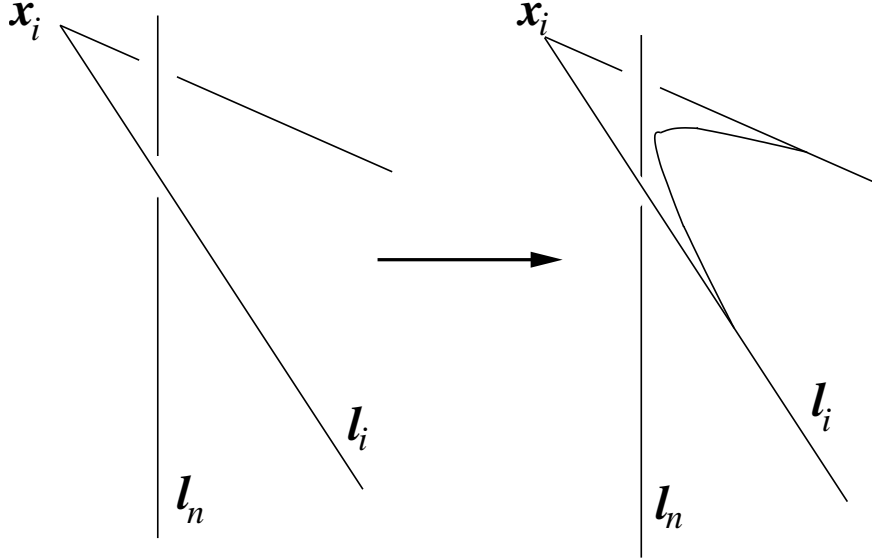


FIG. 6. A situation that should be avoided: before the smoothing of the corner in the point  $\mathbf{x}_i$ , the segment  $\mathbf{l}_n$  was passing under the segment  $\mathbf{l}_i$ . After smoothing, the segment  $\mathbf{l}_i$  has been replaced by an arc of a smooth curve in such a way that the segment  $\mathbf{l}_n$  now passes over that arc, potentially changing the topology of the knot.

by  $\mathbf{l}_1$ . This will require a trivial modification of the procedure that will be presented in the following and that is valid strictly speaking for  $i = 1, \dots, N - 1$ . The parameters  $d_i, d'_i$  are determined starting from  $i = 1$  and then proceeding recursively with the remaining corners in  $\mathbf{x}_2, \mathbf{x}_3, \dots$ . At each step  $i$ , we should check first of all if  $\mathbf{l}_i$  and  $\mathbf{l}_{i+1}$  are parallel or not. If they are parallel, i. e.  $\frac{\mathbf{l}_i \cdot \mathbf{l}_{i+1}}{l_i l_{i+1}} = 1$ , then no action is required because there is no sharp corner and it is possible to pass to the next step  $i + 1$ . In the following, we concentrate in the treatment of the case in which contiguous segments at the  $i$ -th joint are not parallel.

Starting from  $i = 1$ , the first task consists in finding the point  $\mathbf{x}_{k,1}$  belonging to the knot which is the nearest to the vertex  $\mathbf{x}_1$ . The index  $k$  refers to the fact that  $\mathbf{x}_{k,1}$  is lying on a segment  $\mathbf{l}_k$  with  $k \neq 1, 2$ . The restriction  $k \neq 1, 2$  is needed to exclude trivial nearest points belonging to the segments  $\mathbf{l}_1$  and  $\mathbf{l}_2$ .

A way in which the position of  $\mathbf{x}_{k,1}$  may be computed is presented in the Appendix. Let us imagine that  $\mathbf{x}_{k,1}$  is at the distance  $d_{k,1}$  from  $\mathbf{x}_1$ . Then, we choose

$$d_1 = d'_1 = \min \left\{ d_{k,1}, \min \left\{ \frac{l_1}{2}, \frac{l_2}{2} \right\} \right\} \quad (43)$$

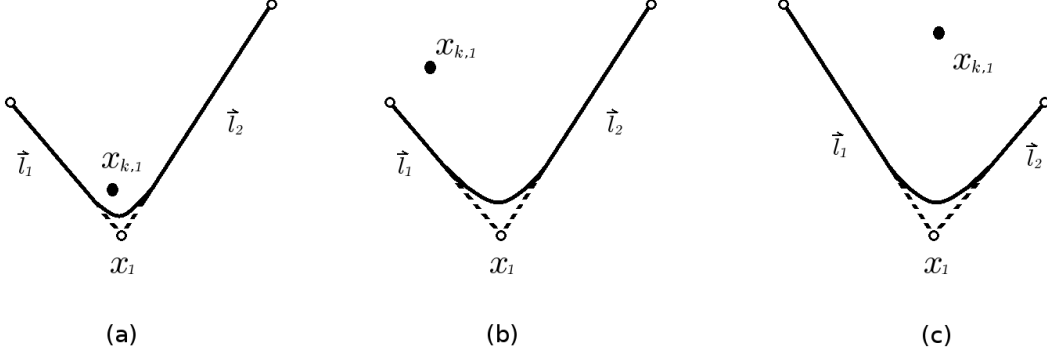


FIG. 7. This series of pictures illustrates the meaning of Eq. (43). In (a) the nearest point  $\mathbf{x}_{k,1}$  to the vertex  $\mathbf{x}_1$  is at a distance  $d_{k,1}$  from  $\mathbf{x}_1$  which is less than  $\min\left\{\frac{l_1}{2}, \frac{l_2}{2}\right\}$ . The length of the segments  $\mathbf{l}_1^+$  and  $\mathbf{l}_2^-$  (represented with dashed lines) is chosen to be  $d_{k,1}$ . These segments, which lie inside a sphere  $S_{\mathbf{x}_1}$  of radius  $d_{k,1}$ , are replaced with smooth curves; (b-c)  $\mathbf{x}_{k,1}$  is at a distance  $d_{k,1}$  from  $\mathbf{x}_1$  which is greater than  $\min\left\{\frac{l_1}{2}, \frac{l_2}{2}\right\}$ . The length of the segments  $\mathbf{l}_1^+$  and  $\mathbf{l}_2^-$  is chosen to be equal to half of the length of the shortest among the segments  $\mathbf{l}_1$  and  $\mathbf{l}_2$ . Next  $\mathbf{l}_1^+$  and  $\mathbf{l}_2^-$  are replaced with smooth curves.

In other words,  $d_1$  is set to be equal to  $d'_1$ . Moreover, depending on the distance  $d_{k,1}$  of the point  $\mathbf{x}_{k,1}$  from  $\mathbf{x}_1$  and on the lengths of the segments  $\mathbf{l}_1, \mathbf{l}_2$ , we can have the three different possibilities displayed in Fig. 7. Fig. 7 (b) refers to the case in which  $l_1 < l_2$  and  $d_{k,1} \geq \frac{l_1}{2}$ . Fig. 7 (c) shows the analogous situation in which  $l_2 \leq l_1$  and  $d_{k,1} \geq \frac{l_2}{2}$ . In both cases, by the prescription (43), the lengths  $d_1, d'_1$  can never be greater than half of the length of the shortest segment between  $\mathbf{l}_1$  and  $\mathbf{l}_2$ . When  $d_{k,1} \leq \min\left\{\frac{l_1}{2}, \frac{l_2}{2}\right\}$ , we have the situation depicted in Fig. 7 (a). Let us notice that the values  $d_1, d'_1$  are selected in such a way that both subsegments  $\mathbf{l}_1^+$  and  $\mathbf{l}_2^-$ , together with the smooth arc of curve replacing them, lies inside a sphere  $S_{\mathbf{x}_1}$  of radius  $d_1$ . This sphere contains the point  $\mathbf{x}_{k,1}$ . Since  $\mathbf{x}_{k,1}$  is the point on the knot which is nearest to  $\mathbf{x}_1$  excluding the points on the segments  $\mathbf{l}_1$  and  $\mathbf{l}_2$ , this implies that no unwanted segment is contained in  $S_{\mathbf{x}_1}$ . Thus, dangerous situations such as those presented in Fig. 6 are not possible.

Now we suppose that all the values of  $d_j = d'_j$  have been computed up to  $j < i$ . Implicitly, excluding corners in which the segments  $\mathbf{l}_{j-1}, \mathbf{l}_j$  are parallel, we should assume that the subsegments  $\mathbf{l}_j^\pm$  with  $j < i$  and  $\mathbf{l}_i^-$  have already been replaced by the smooth arcs of curves of Eqs. (39–40). We also assume that the smoothing procedure has been carried in such a



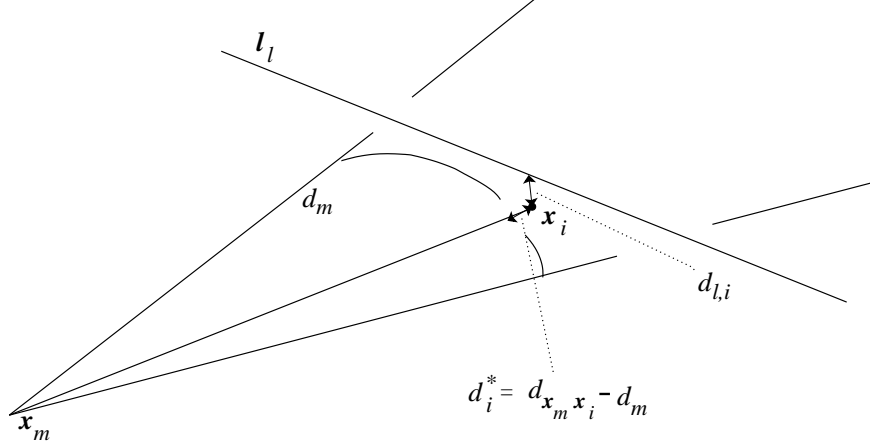


FIG. 8. This picture explains the meaning of the quantity  $d_i^*$  appearing in Eq. (44). It shows also the procedure with which the radius  $d_i$  of the sphere  $S_{x_i}$  is chosen.

way that, for  $j < i - 1$ , the arcs substituting the subsegments  $l_j^+, l_{j+1}^-$  are inside a sphere  $S_{x_j}$  of radius  $d_j$  and no other part of the knot after the replacements made so far is contained in this sphere. The same statement should be true in the case  $j = i - 1$  too, in which the sphere  $S_{x_{i-1}}$  of radius  $d_{i-1}$  is allowed to contain only the arcs of curves which replaced the subsegments  $l_{i-1}^+, l_i^-$ .

At this point we have to deal with the corner corresponding to the vertex in  $x_i$ . As we did for the first corner in  $x_1$ , we determine the position  $x_{l,i}$  of the point which is nearest to  $x_i$  and does not belong to  $l_i$  or  $l_{i+1}$ . Let's suppose that  $x_{l,i}$  lies on the segment  $l_l$  with  $l \neq i, i + 1$  and is at a distance  $d_{l,i}$  from  $x_i$ . We have also to be sure that no point of the spheres  $S_{x_k}$  with  $k = 1, \dots, i - 1$  corresponding to a corner that has already been substituted is at a distance from  $x_i$  which is smaller than  $d_{l,i}$ . To this purpose we compute the minimal distance  $d_i^*$  from  $x_i$  to these spheres:

$$d_i^* = \min_{k=1, \dots, i-1} \{d_{l,i}, d_{x_k x_i} - d_k\} \quad (44)$$

The meaning of  $d_i^*$  is illustrated in Fig. 8. The following three situations should be treated separately:

1.  $l > i$  and  $d_i^* \geq d_{l,i}$ .
2.  $l < i$  and  $d_i^* \geq d_{l,i}$ .
3.  $d_i^* < d_{l,i}$ .

In the first case, the substituted parts of the knot are at a distance  $d_i^*$  which is greater than  $d_{l,i}$ . As a consequence, the segment  $\mathbf{l}_l$  contains the point  $\mathbf{x}_{l,i}$  which is among all points of the knot the nearest one to  $\mathbf{x}_i$ . Moreover,  $\mathbf{l}_l$  has not yet been affected by the smoothing procedure. It is thus possible to proceed as we did for the first corner  $\mathbf{x}_1$ . The second case is more complicated. The point  $\mathbf{x}_{l,i}$  on the segment  $\mathbf{l}_l$  is nearer to  $\mathbf{x}_i$  than any other point lying on the other segments or on the parts of the knot that have already been replaced, but the segment  $\mathbf{l}_l$  has been affected by the smoothing procedure. This means that  $\mathbf{x}_{l,i}$  could have been mapped to a new point  $\mathbf{x}'_{l,i}$  and it is no longer trivial to determine which is the new nearest point to  $\mathbf{x}_i$ . Three subcases are possible, see Fig. 9 for a visual representation:

2.-a)  $\mathbf{x}_{l,i}$  is near the point  $\mathbf{x}_{l-1}$  within the distance  $d_{l-1}$ , i. e.  $\mathbf{x}_{l,i}$  lies on the segment  $\mathbf{l}_l^-$ . This implies that for sure  $\mathbf{x}_{l,i}$  has been already mapped into the point  $\mathbf{x}'_{l,i}$  located on the arc of the smooth curve that replaced  $\mathbf{l}_l^-$ . What we know is that both segment  $\mathbf{l}_l^-$  and the arc of the smooth curve replacing it are inside the sphere  $S_{\mathbf{x}_{l-1}}$  of radius  $d_{l-1}$ . The radius  $d_i$  of the sphere  $S_{\mathbf{x}_i}$  surrounding  $\mathbf{x}_i$  should be chosen in such a way that  $S_{\mathbf{x}_{l-1}}$  and  $S_{\mathbf{x}_i}$  do not penetrate into each other. We should also avoid that  $S_{\mathbf{x}_i}$  penetrates inside any other sphere  $S_{\mathbf{x}_k}$  with  $k < i$ . Due to the condition  $d_i^* \geq d_{l,i}$ , which is valid in this subcase, this last requirement is matched if the following inequality is satisfied:

$$d_i, d'_i \leq d_{l,i} \quad (45)$$

Let  $d_{\mathbf{x}_{l-1}\mathbf{x}_i}$  be the distance between  $\mathbf{x}_{l-1}$  and  $\mathbf{x}_i$ . Since in our construction  $d_{l-1}$  can be only less or equal to the minimal distance between  $\mathbf{x}_{l-1}$  and any segment  $\mathbf{l}_n$  with  $n \neq l-1, l$ , it is possible to conclude that:

$$d_{\mathbf{x}_{l-1}\mathbf{x}_i} \geq d_{l-1} \quad (46)$$

If  $d_{l-1}$  is strictly smaller than  $d_{\mathbf{x}_{l-1}\mathbf{x}_i}$ , then the following inequalities hold:

$$0 < d_{\mathbf{x}_{l-1}\mathbf{x}_i} - d_{l-1} < d_{l,i} \quad (47)$$

The left inequality is a trivial consequence of our settings. To prove that  $d_{\mathbf{x}_{l-1}\mathbf{x}_i} - d_{l-1} < d_{l,i}$ , we remember that, under the present assumptions:

$$0 < d_{\mathbf{x}_{l,i}\mathbf{x}_{l-1}} < d_{l-1} \quad (48)$$

where  $d_{\mathbf{x}_{l,i}\mathbf{x}_{l-1}}$  denotes the distance between the points  $\mathbf{x}_{l,i}$  and  $\mathbf{x}_{l-1}$ . Eq. (48) simply states the fact that the point  $\mathbf{x}_{l,i}$  lies in the subsegment  $\mathbf{l}_l^-$  whose length is  $d_{l-1}$ . Moreover, using the properties of the norm expressing the distances on Euclidean spaces, it turns out that

$$d_{\mathbf{x}_{l-1}\mathbf{x}_i} \leq d_{\mathbf{x}_{l,i}\mathbf{x}_{l-1}} + d_{l,i} \quad (49)$$

Applying the second inequality appearing in Eq. (48) to (49), we obtain that  $d_{\mathbf{x}_{l-1}\mathbf{x}_i} - d_{l-1} < d_{l,i}$ , thus proving Eq. (47). As a consequence, a sphere  $S_{\mathbf{x}_i}$  of radius  $d_{\mathbf{x}_{l-1}\mathbf{x}_i} - d_{l-1}$  around the point  $\mathbf{x}_i$  will never contain any point of the knot apart from the points belonging to the segments  $\mathbf{l}_i$  and  $\mathbf{l}_{i+1}$ . This is due to Eq. (47), which states that the radius of  $S_{\mathbf{x}_i}$  is smaller than the distance  $d_{l,i}$  between  $\mathbf{x}_i$  and the nearest point to  $\mathbf{x}_i$ . Thus, the condition (45), which is sufficient to avoid points of contacts between  $S_{\mathbf{x}_i}$  and the spheres  $S_{\mathbf{x}_k}$  of radii  $d_k$  for  $k = 1, \dots, i-1$  and  $k \neq l-1$ , is fulfilled. Moreover, when  $k = l-1$ , by construction the sphere  $S_{\mathbf{x}_{l-1}}$  has only one point of contact with  $S_{\mathbf{x}_i}$ , see Fig. 9. Thus, it is possible to safely choose  $d_i$  and  $d'_i$  as follows:

$$d_i = d'_i = \min \left\{ d_{\mathbf{x}_{l-1}\mathbf{x}_i} - d_{l-1}, \min \left\{ \frac{l_i}{2}, \frac{l_{i+1}}{2} \right\} \right\} \quad (50)$$

With this choice, in fact, no dangerous crossing of lines may occur between the arcs of curves already replaced and the subsegments that have still to be treated, see also Fig. 9 for a visual representation of the situation.

We are left with the particular case  $d_{\mathbf{x}_{l-1}\mathbf{x}_i} = d_{l-1}$ , which can never happen under the present hypothesis that  $l < i$  and  $d_i^* \geq d_{l,i}$ . As a matter of fact, if  $d_{\mathbf{x}_{l-1}\mathbf{x}_i} = d_{l-1}$ , the quantity  $d_i^*$  defined in Eq. (44) is zero and, as a consequence,  $d_i^* < d_{l,i}$ , because  $d_{l,i}$  can never vanish since the segments  $\mathbf{l}_l$  and  $\mathbf{l}_i$  are not allowed to intersect. The situations in which  $d_i^* = 0$  will be treated in the next point dedicated to case 3 of page 17.

2.-b)  $\mathbf{x}_{l,i}$  is near the point  $\mathbf{x}_l$  within a distance which is less than  $d_l$ , i. e. it lies on the segment  $\mathbf{l}_l^+$  that has already been substituted. In that case the procedure to determine  $d_i, d'_i$  is analogous to that used in the case 2.-a).

2.-c)  $\mathbf{x}_{l,i}$  is on the subsegment  $\mathbf{l}_l^0$ , In that case there is no problem because this subsegment has not been replaced with an arc of a curve and we may proceed by taking:

$$d_i = d'_i = \min \left\{ d_{l,i}, \min \left\{ \frac{l_i}{2}, \frac{l_{i+1}}{2} \right\} \right\} \quad (51)$$

Finally, we deal with the case 3 of page 17. We distinguish the following two subcases:

$$d_i = d'_i = \min \left\{ d_i^*, \min \left\{ \frac{l_i}{2}, \frac{l_{i+1}}{2} \right\} \right\} \quad (52)$$

3-b)  $d_i^* = 0$ . As a consequence, there exist a sphere  $S_{\mathbf{x}_m}$  of radius  $d_m$  centered at the point  $\mathbf{x}_m$  for some value of  $m \leq i - 1$  such that  $\mathbf{x}_i$  lies on the border of this sphere. On the other side, no point of the knot may be nearer to  $\mathbf{x}_i$  than  $\mathbf{x}_{l,i}$ , which is at the distance  $d_{l,i} > d_i^* = 0$  from  $\mathbf{x}_i$ . Yet, it may happen that there exists another sphere, let say

$S_{\mathbf{x}_n}$ , with  $n \leq i-1$  and  $n \neq m$  centered at a point  $\mathbf{x}_n$ , such that the distance between the border of  $S_{\mathbf{x}_n}$  and  $\mathbf{x}_i$  is less than  $d_{l,i}$ . To take into account this case, it is useful to compute also the quantity  $d_i^{*'}^{31}$ :

$$d_i^{*'} = \min_{\substack{k=1,\dots,i-1 \\ k \neq m}} \{d_{l,i}, d_{\mathbf{x}_k \mathbf{x}_i} - d_k\} \quad (53)$$

At this point a possible way to define  $d_i$  and  $d'_i$  consists in putting

$$d_i = d'_i = \min \left\{ \min \left\{ d_i^{*'}, \frac{d_k}{2} \right\}, \min \left\{ \frac{l_i}{2}, \frac{l_{i+1}}{2} \right\} \right\} \quad (54)$$

and to decrease the value of the radius of the sphere  $S_{\mathbf{x}_k}$  as follows:

$$d_k \longrightarrow \frac{d_k}{2} \quad (55)$$

Clearly, the choice of  $d_i, d'_i$  given above does not allow crossings of the lines that can change the type of the knot.

Let us stress that, within the procedure illustrated above, at each stage  $i$  the arcs of the curves replacing the corners are always contained inside a sphere centered at the  $i$ -th corner. The spheres corresponding to different corners never intersect themselves apart from one point on their surfaces which may be in common. In this way, there is no possibility that the trajectory of the knot crosses itself during the replacement of the sharp corners causing unwanted changes of the topology of the knot. The result is that the trajectory of the discrete knot becomes a  $G^1$ -curve, which is the condition sufficient in order to compute the Vassiliev knot invariant of degree 2 without the systematic errors related to the presence of the sharp corners. The only drawback is that the parameters  $d_i$ , and thus the portions of the corners that have been replaced, become smaller and smaller when the value of  $i$  increases. This is a drawback because an extensive Monte Carlo sampling procedure is required in order to evaluate  $\varrho(C)$  with a good approximation if the arcs of curves replacing the corners exhibit sharp turns.

The method explained above is somewhat complicated, but this is only because we are considering very general discrete knots, defined off or on lattice and with segment of different lengths. On a lattice, many simplifications are possible. For instance, on a simple cubic lattice one may always choose  $d_i = d'_i = \frac{l_i}{2}$  without the risk of changing the topology of the knot. In that case it is easy to check that Eqs. (39–40) reduce to the equation:

$$\mathbf{X}_i^\pm(S) = (1 - \sin(\theta_0^\pm(S))) \mathbf{l}_i^+ + (1 - \cos(\theta_0^\pm(S))) \mathbf{l}_{i+1}^- + \mathbf{x}_i \quad (56)$$

where

$$\theta_0^+(S) = \left( S - [S] - \frac{1}{2} \right) \frac{\pi}{2} \quad (57)$$

and

$$\theta_0^-(S) = \left( S - [S] + \frac{1}{2} \right) \frac{\pi}{2} \quad (58)$$

Similar simplifications occur in the ansatz of Eqs. (39–40) in the particular case (off and on lattice) in which all the segments have the same length and the  $d_i$ 's coincide with the  $d'_i$ 's.

Finally, after the values  $d_i, d'_i$  are computed for all the corners, the points on the knot are sampled using the following prescriptions:

**Step 1:** Pick up a random number  $S$  in the interval  $[0, N]$ . These random variables are necessary in order to generate the points  $\mathbf{X}(S)$  needed for the Monte Carlo procedure. The value of  $S$  identifies a segment  $\mathbf{l}_i$  with  $i = [S] + 1$  and end points  $\mathbf{x}_i = \mathbf{X}([S] + 1)$  and  $\mathbf{x}_{i-1} = \mathbf{X}([S])$ . This procedure works also for  $i = 1$  provided the point  $\mathbf{x}_0$  is identified with  $\mathbf{x}_N$ .

**Step 2:** We assume that the curve is oriented in such a way that the  $i$ -th segment  $\mathbf{l}_i$  is coming before the segment  $\mathbf{l}_{i+1}$ . Now we have to check if one of the following three conditions are satisfied:

$$0 \leq S - [S] < \frac{d'_{i-1}}{l_i} \quad (59)$$

$$\frac{d'_{i-1}}{l_i} \leq S - [S] < \frac{l_i - d_i}{l_i} \quad (60)$$

$$\frac{l_i - d_i}{l_i} \leq S - [S] < 1 \quad (61)$$

The first condition (59) identifies the subsegment  $\mathbf{l}_i^-$ , the second condition (60) the subsegment  $\mathbf{l}_i^0$  and the third one (61) the subsegment  $\mathbf{l}_i^+$ .

**Step 3:** When condition (59) is fulfilled, verify if the relation

$$\frac{\mathbf{l}_{i-1}^+ \cdot \mathbf{l}_i^-}{l_{i-1}^+ l_i^-} = -1 \quad (62)$$

is satisfied. If yes, the segments  $\mathbf{l}_{i-1}^+$  and  $\mathbf{l}_i^-$  around the corner  $\mathbf{x}_{i-1}$  are antiparallel and there is no sharp corner to be smoothed up. In that case the smoothed curve coincides with the old one and the parametrization given in Eqs. (15–16) is still valid. If instead

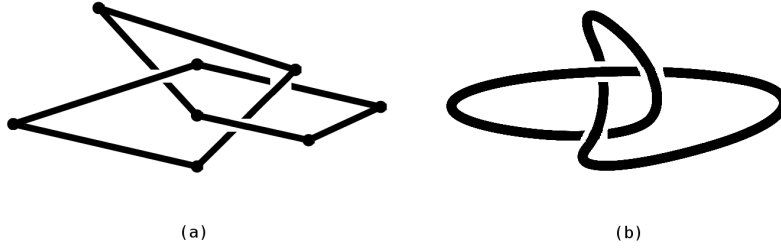


FIG. 10. A knot  $3_1$  with minimal length defined off lattice before and after the smoothing procedure.

the segments  $\mathbf{l}_{i-1}^+$  and  $\mathbf{l}_i^-$  are not antiparallel, then we have to use the prescription of Eq. (40), which is valid on  $\mathbf{l}_i^-$  after the replacement  $i \rightarrow i - 1$ . The point  $\mathbf{X}(S)$  is projected onto the point  $\mathbf{X}_i^-(S)$  with the help of Eq. (40). A similar procedure is adopted when condition (61) is true. In that case the condition of being antiparallel is concerning the segments  $\mathbf{l}_i^+$  and  $\mathbf{l}_{i+1}^-$ :

$$\frac{\mathbf{l}_i^+ \cdot \mathbf{l}_{i+1}^-}{l_i^+ l_{i+1}^-} = -1 \quad (63)$$

If it turns out that  $\mathbf{l}_i^+$  and  $\mathbf{l}_{i+1}^-$  are not antiparallel, then the point  $\mathbf{X}(S)$  should be mapped using the curve in Eq. (39). Finally, when condition (60) is satisfied, we are on the subsegment  $\mathbf{l}_i^0$  away from any corner. As a consequence, for the values of  $S$  in the interval  $[\frac{d'_{i-1}}{l_i}, \frac{l_i - d_i}{l_i}]$ , it is possible to apply the old parametrization of Eqs. (15–16).

An example of curve describing a discrete knot  $3_1$  off lattice before and after the smoothing procedure is shown in Fig. 10.

The smoothing procedure illustrated above has been applied to many examples of different knots of various lengths. It delivers values of the Vassiliev invariant of degree 2 which are approaching the exact value with a precision that increases with the increase of the number of samples used in the Monte Carlo integration algorithm. In Table I we report for instance the case of a knot  $3_1$  with 24 segments computed using gradually increasing numbers of samples.

Table II illustrates how the presence of the sharp corners affects the calculations of  $\varrho(C)$ . In the second column of Table II, the outcome  $\varrho_a(C)$  of the analytical computation of  $\varrho(C)$  is provided for several knots with number of segments  $N = 90$ . Within the given errors,

$n$	$\varrho(C)$
$10^6$	$1.9096 \pm 0.0991$
$10^7$	$1.9179 \pm 0.0326$
$10^8$	$1.9170 \pm 0.0095$
$10^9$	$1.9168 \pm 0.0032$

TABLE I. Computation of the knot invariant  $\varrho(C)$  for the knot  $3_1$  with 24 segments on a simple cubic lattice. The results of the numerical calculation of  $\varrho(C)$  are displayed for different values of the number of samples  $n$  used in the Monte Carlo integral procedure. As it can be seen, by gradually increasing  $n$ , the numerical values of  $\varrho(C)$  asymptotically approach the analytical value of the Vassiliev knot invariant of degree 2 which, in the case of the knot  $3_1$ , is approximately equal to 1.9167.

the values  $\varrho_{sp}(C)$  obtained by Monte Carlo integration after the smoothing procedure (sp) are in agreement with the analytical results, see the third column of Table II. We are also reporting the upshot of the calculations performed without the smoothing procedure, see the values of  $\varrho_{ns}(C)$  in the fourth column of Table II. The differences between  $\varrho_{sp}(C)$  and  $\varrho_{ns}(C)$  show that indeed the presence of sharp corners in the case of discrete knots does not allow the correct evaluation of the knot invariant  $\varrho(C)$ .

## V. SPEEDING UP THE MONTE CARLO ALGORITHM

The computation of the Vassiliev invariant of degree 2 by Monte Carlo methods is much more convenient than by traditional numerical techniques. For instance, in order to evaluate  $\varrho(C)$  with sufficient precision in the case of knots of length  $L \leq 120$ , a few millions of samples are enough. This is a quite good performance if we take into account that, for  $N = 120$  the total volume to be checked is  $\frac{120^4}{24} \sim 9 \cdot 10^6$ . If a very high precision is required or  $N$  is large, the sampling procedure can be easily parallelized on a computer. Still, the numerical evaluation of  $\varrho(C)$  becomes challenging especially in the case of knots consisting of a large number of segments and it is advisable to adopt some strategy in order to reduce the calculation time. Let us notice at this point that, in practical applications, knot invariants are mainly used in order to make assessments on the topological configuration of a knot



knot type	$\varrho_a(C)$	$\varrho_{sp}(C)$	$\varrho_{ns}(C)$	$n_{sc}$
0 <sub>1</sub>	$-\frac{1}{12}$	$-0.0839 \pm 0.0332$	$+0.5526 \pm 0.0569$	77
3 <sub>1</sub>	$+\frac{23}{12}$	$+1.9170 \pm 0.0553$	$+2.4781 \pm 0.0465$	68
4 <sub>1</sub>	$-\frac{25}{12}$	$-2.0847 \pm 0.0533$	$-1.5214 \pm 0.0845$	68
5 <sub>1</sub>	$+\frac{71}{12}$	$+5.9174 \pm 0.0653$	$+6.4523 \pm 0.0845$	65
6 <sub>1</sub>	$-\frac{49}{12}$	$-4.0856 \pm 0.0723$	$-3.5717 \pm 0.1007$	62
7 <sub>1</sub>	$+\frac{143}{12}$	$+11.9173 \pm 0.0652$	$+12.4258 \pm 0.1217$	62
8 <sub>1</sub>	$-\frac{73}{12}$	$-6.0822 \pm 0.0529$	$-5.6380 \pm 0.0774$	54
9 <sub>1</sub>	$+\frac{239}{12}$	$+19.9158 \pm 0.0855$	$+20.4041 \pm 0.1579$	59

TABLE II. This table provides the values of the Vassiliev knot invariant of degree 2 for the knots 0<sub>1</sub>, 3<sub>1</sub>, 4<sub>1</sub>, 5<sub>1</sub>, 6<sub>1</sub>, 7<sub>1</sub>, 8<sub>1</sub> and 9<sub>1</sub>.  $\varrho_a(C)$  denotes the analytical value of the knot invariant.  $\varrho_{sp}(C)$  refers to the results of the computation of the knot invariant obtained after performing the smoothing procedure described in Section IV.  $\varrho_{ns}(C)$  is instead the value of the knot invariant derived without the smoothing procedure. The data of  $\varrho_{sp}(C)$  and  $\varrho_{ns}(C)$  have been computed using the same number of samples, which varies depending on the kind of knot. Finally,  $n_{sc}$  is the number of sharp corners contained in the knot before the smoothing procedure.

which is a priori unknown. To that purpose, it is not necessary to evaluate  $\varrho(C)$  beyond a certain precision, as it will be evident from the following discussion. First of all, let's recall the fact that there is no knot invariant that is able to distinguish unambiguously all different types of knots. The Vassiliev invariant of degree 2 is not an exception to this rule, but still may be considered as a relatively powerful knot invariant. For example, it is able to distinguish uniquely the knots 9<sub>1</sub> and 10<sub>3</sub> from all other knots up to ten crossings. Of course, there are many knots for which the second coefficient of the Conway polynomial  $a_2(C)$  is the same. This implies that  $\varrho(C)$ , which is related to  $a_2(C)$  by Eq. (10), can at most be used to distinguish classes of knots having different values of  $a_2(C)$ . A nice characteristic of  $\varrho(C)$  consists in the fact that, if two knots  $C$  and  $C'$  can be resolved by it, then the condition

$$|\varrho(C) - \varrho(C')| \geq 2 \quad (64)$$

is always satisfied. As a consequence, in order to ascertain the difference between two knots with the help of a Monte Carlo calculation of  $\varrho(C)$ , it is not necessary to push the standard

deviation  $\sigma$  of the numerical calculation of  $\varrho(C)$  below a given threshold value  $\sigma_{threshold}$ . For instance, we can choose:

$$\sigma_{threshold} = \frac{1}{6.11} \sim 0.16 \quad (65)$$

If  $\sigma = \sigma_{threshold}$ , in fact, the probability that the Monte Carlo evaluation of  $\varrho(C)$  gives a result within an error of  $\pm 1$  or greater is of the order  $1 \cdot 10^{-9}$ , i. e. this event is very unlikely. If two knots  $C$  and  $C'$  are distinguishable by using the Vassiliev invariant of degree 2, then, due to Eq. (65), this precision is more than enough to state if  $C$  and  $C'$  are different or not with a satisfactory confidence level. The possibility of putting a lower cutoff to the standard deviation as in Eq. (65) is very helpful in practical calculations because, in order to decrease the standard deviation, it is necessary to increase the number of samples used in the Monte Carlo integration method. Of course, this leads to a consistent increase of the calculation time. In fact, the time  $\tau$  necessary for computing  $\varrho(C)$  scales linearly with the number of samples  $n$ , but an increasing of  $n$  by a factor  $\lambda > 1$  produces an improvement of  $\sigma$  only by a factor  $\frac{1}{\sqrt{\lambda}}$ , i. e.  $\sigma \longrightarrow \frac{\sigma}{\sqrt{\lambda}}$ . We have checked that this scaling law, that is predicted in the case of gaussian distributions, is actually verified in the present context.

Besides the standard deviation, another important factor which determines the computation time  $\tau$  is the number  $N$  of segments (or equivalently the number of arcs of  $G^1$ -trajectories) in which the trajectory of the knot is realized. Due to the presence of a quadruple contour integral in  $\varrho_2(C)$ , see Eqs. (3) and (5),  $\tau$  scales with respect to  $N$  according to the fourth power, i. e.  $\tau \propto N^4$ . We stress the fact that  $\tau$  depends on the number of points  $N$  and not on the knot length  $L$ . The length of the knot depends in fact on the lengths  $l_i$  of the segments  $\mathbf{l}_i$  for  $i = 1, \dots, N$ . In turn, the  $l_i$ 's can be made arbitrarily small by the rescalings

$$l_i \longrightarrow l'_i = \eta l_i \quad i = 1, \dots, N \quad (66)$$

where  $\eta$  is any real parameter such that  $0 < \eta < 1$ . In fact, rescalings of this kind do not affect the value of  $\varrho(C)$ , which is a scale invariant quantity. To prove the statement that  $\tau \propto N^4$ , it is sufficient to decompose, as it has been done in Ref.<sup>17</sup>, the quadruple integral in Eq. (3) into a quadruple sum of contour integrals in which the contours are the segments  $\mathbf{l}_i$  themselves. With the rescalings of Eq. (66) it is then possible to reduce the lengths of these segments to infinitesimal quantities. As a consequence, the contour integrals over the segments  $\mathbf{l}_i$  can be computed exactly. In this way, only the quadruple sum over the indexes

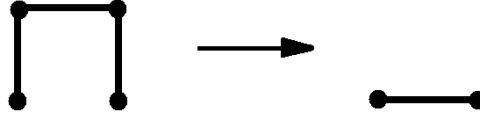


FIG. 11. Reduction to a single segment of an element of the discrete knot composed by three consecutive segments such that its ends are at a distance equal to the unit size on a simple cubic lattice. The topology of the knot is not affected by this reduction.

labeling the segments remains which contains exactly  $\frac{N^4}{24}$  terms. For knots composed by a large number of segments, this implies that the number of samples necessary for obtaining a satisfactory result from the Monte Carlo integration algorithm becomes prohibitively high. This problem can be partially avoided by adopting procedures that are able to shorten a given discrete knot reducing its number of segments without changing its topology. In the following, a few such procedures will be proposed, most of them valid on a simple cubic lattice before applying the smoothing procedure:

1. For a general discrete polymer, it is always possible to group together contiguous segments that are parallel.
2. On a simple cubic lattice, configurations of three segments whose ends are at a distance equal to the size of a lattice edge can be easily substituted by one segment as shown in Fig. 11. This reduces the length of the knot by two segments every time this configuration is encountered.
3. Always on a simple cubic lattice it is possible to group together two or three contiguous segments in a single one, see Figs. 12 and 13. We note that the first substitution in Fig. 13 can cause intersections between two segments after the grouping and should be treated with some care.

Other algorithms to decrease the size of a knot can be found in Refs.<sup>26</sup> and<sup>27</sup>, where the KMT radiation scheme has been introduced.

Finally, we show yet another strategy which can be used to speed up the Monte Carlo procedure when the knot invariant is needed to assess the topology of a knot after a random transformation that can be in principle not topology-preserving. We will assume that

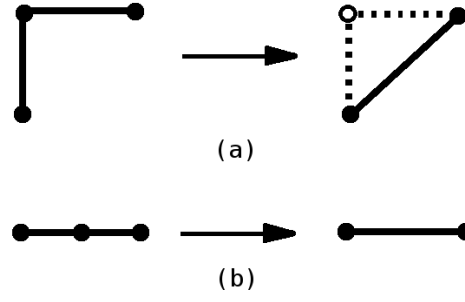


FIG. 12. This figure displays the possible configurations on a simple cubic lattice of two contiguous segments and their substitution with a single segment. The topology of the knot is left unchanged after the substitution.

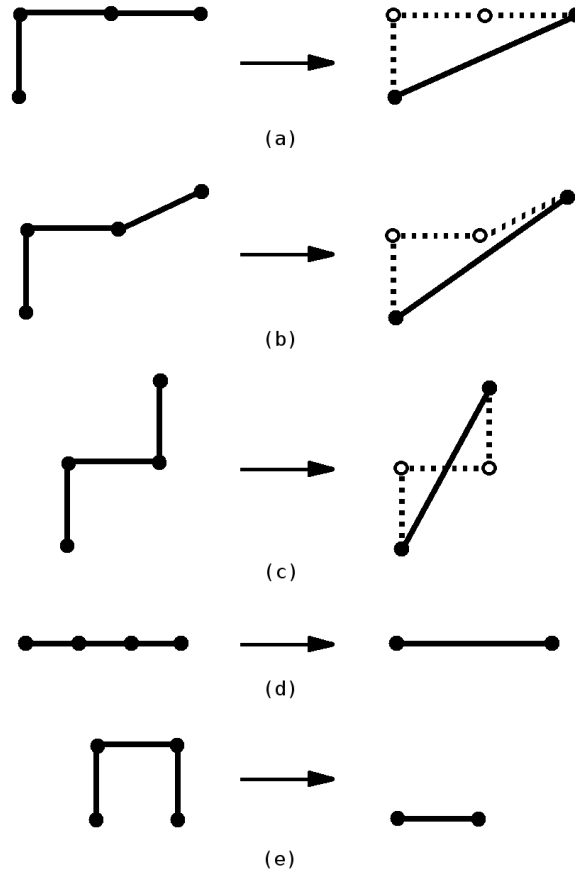


FIG. 13. This figure displays the possible configurations on a cubic lattice of three contiguous segments and their substitution with a single segment.

the random transformation involves  $K$  contiguous segments, where  $0 \leq K \leq N$ . Instead of calculating the whole knot invariant  $\varrho(C)$ , it is much better to compute the difference  $\Delta\varrho(C) = \varrho(C_T) - \varrho(C_R)$ . Here  $C_R$  is the polymer conformation before the transformation. By hypothesis,  $C_R$  is in the desired topological configuration.  $C_T$  denotes instead the conformation after the transformation. The problem is to ascertain if the new knot  $C_T$  is topologically equivalent to  $C_R$ . Clearly, if  $\varrho(C)$  would be a perfect topological invariant, this would be true only if  $\varrho(C_T) - \varrho(C_R) = 0$ . Unfortunately,  $\varrho(C)$  is not able to distinguish unambiguously two different topological configurations. However,  $\varrho(C)$  is a quite powerful knot invariant. Moreover, the probability to pass with a single random transformation from a knot  $C_R$  to a knot  $C_T$  such that  $C_R$  and  $C_T$  are topologically inequivalent but are still characterized by the same value of the Vassiliev knot invariant of degree 2 seems not to be quite high. For this reason it is licit to expect that  $C_T$  and  $C_R$  are very likely to be of the same topological type if the result of the numerical evaluation of the difference  $\Delta\varrho(C) = \varrho(C_T) - \varrho(C_R)$  gives a nearly vanishing result. The advantage of considering  $\Delta\varrho(C)$  instead of computing the whole value of the knot invariant for  $C_T$  is that in this way we can ignore the part of the knot that has remained unchanged after the transformation.

To realize that this strategy is convenient, we limit ourselves to the calculation of  $\varrho_2(C)$ , which is the contribution to  $\varrho(C)$  that requires the biggest computational effort. From Eq. (23), it turns out that to estimate the value of  $\varrho_2(C)$ , the volume to be explored via the Monte Carlo sampling procedure is equal to  $N^4/24$ . If the number of the changed segments is  $K$ , then at the leading order the number of terms involving only segments that have not been affected by the transformation is equal to  $(N - K)^4/24$ . As a consequence, the number of summands to be taken into account in the evaluation of the difference  $\varrho(C_T) - \varrho(C_R)$  is

$$\begin{aligned} S_K &= \frac{N^4}{24} - \frac{(N - K)^4}{24} \\ &= \frac{NK^3}{6} - \frac{N^2K^2}{4} + \frac{N^3K}{6} - \frac{K^4}{24} \end{aligned} \quad (67)$$

Clearly, the minimum of  $S_K$  with respect to  $K$  occurs when  $K = 4$  (we do not consider here transformations with less than 4 segments). Due to the fact that the derivative of  $S_K$  with respect to  $K$  in the range  $0 \leq K \leq N$  is always positive, because  $\frac{dS_K}{dK} = \frac{(N-K)^3}{6} > 0$ , it turns out that  $S_K$  grows with  $K$  until it reaches its maximum when  $K = N$  (transformations of more than  $N$  segments do not make sense). If  $K$  is small with respect to  $N$ , Eq. (67) shows that the volume to be explored in the computation of  $\Delta\varrho_2(C)$  is much less than that

needed to obtain  $\varrho_2(C)$ . For instance, when  $K = N/5$ , we obtain:

$$S_K = 0.5904 \times \frac{N^4}{24} \quad (68)$$

so that only 60% of the original volume  $\frac{N^4}{24}$  should be considered. In the best case,  $K = 4$ , instead,

$$S_4 \sim \frac{2N^3}{3} \quad (69)$$

which implies an enormous gain in speed.

## VI. CONCLUSIONS

In this work an algorithm to compute the Vassiliev invariant of degree 2  $\varrho(C)$  for any knot  $C$  has been provided. Particular attention has been devoted to discrete knots whose trajectories consist of segments connected together at their ends forming  $C^0$ -curves in the space. This case is relevant in numerical simulations, where knots are forcefully discretized and represented as  $C^0$ -curves. The Vassiliev invariant of degree 2 is probably the simplest knot invariant that can be defined in terms of multiple integrals computed along the contour of the knot itself. For this reason, there are chances that in the future this invariant will play for knots the same role played by the Gauss linking number in numerical studies of links formed by ring-shaped quasi one-dimensional objects. A suitable parametrization of discrete knots has been introduced, see Eqs. (11–16) and the problem of computing the multiple contour integrals has been tackled using the Monte Carlo integration scheme summarized by the general equation (24). In principle, using the scale invariance of  $\varrho(C)$ , it is possible to reduce arbitrarily the length of the knot, because a change of scale does not alter its topology. However, even in the best case in which the lengths of the segments become infinitesimal, so that the integration over them can be easily approximated, standard methods require the computation of a sum over  $\frac{N^4}{24} + \frac{N^3}{6}$  terms in order to obtain the value of  $\varrho(C)$ , as shown in<sup>17</sup> and in the previous Section. With the Monte Carlo integration a considerably smaller number of samples is necessary in order to evaluate  $\varrho(C)$  with a satisfactory approximation. For this reason, the standard integration methods like the Simpson's rule are decidedly slower as it is pointed out by the example provided at the beginning of Section V of a knot with 120 segments. Further refinements of the naive Monte Carlo integration scheme

presented in Section III are difficult to be implemented or do not increase substantially the speed of the computations. For instance, the division of the integration domain, which is recommended as one of the strategies to improve the sampling efficiency, did not lead to significant improvements. On the other side, it is not easy to guess which distribution of the values of the integration variables could be suitable in order to enhance the sampling procedure.

In the computations of  $\varrho(C)$  for discrete knots consisting of a set of segments, we have found that the results never coincide with the analytical values. This is expected because of the sharp corners at the points where the segments join together. There is some correlation between the number of these corners and the systematic error in the evaluation of  $\varrho(C)$  that apparently depends on the type of the knot and the number of its segments  $N$ . However, to establish a general relation between that systematic error and  $N$  which could be valid for every knot has not been possible. To solve the problem of the sharp corners, a procedure for the smoothing of discrete knots has been presented in Section IV. This procedure transforms the discrete knot into a  $G^1$ -curve. After the smoothing, it has been possible to evaluate  $\varrho(C)$  with an arbitrary precision by gradually increasing the number of samples used in the Monte Carlo integration of the multiple integrals entering the definition of  $\varrho(C)$ , see for example Table I. Despite the advantages of the adopted Monte Carlo method with respect to the traditional integration techniques, the calculation of  $\varrho(C)$  becomes challenging when the number of segments composing the knot is large. For certain physical applications of the knot invariant  $\varrho(C)$ , we show that the time necessary for its evaluation, which approximately scales as the fourth power of  $N$  when  $N$  is large, can be reduced in such a way that scales with the third power of  $N$ , see Eq. (69). Moreover, we present an algorithm to reduce the number of segments of a knot defined on a cubic lattice by a factor three without changing the topology. After this reduction, the knot is no longer defined on a lattice, but still the general smoothing procedure of Section IV and the provided Monte Carlo integration scheme of Section III can be applied in order to obtain the value of  $\varrho(C)$ . To give an idea of the efficiency of the methods for reducing the number of segments explained in Section V, in the case of a knot with  $N = 1000$  originally constructed on a simple cubic lattice, the number of segments in the final configuration obtained after the treatment ranges between 255 and 300 depending on the initial shape of the knot. Finally, it is important to notice that, in order to distinguish the topology of different knots, it is not necessary to achieve a

standard deviation that is lower than the threshold value given in Eq. (65). In this case, in fact, the probability that one knot could be confused with a topologically inequivalent one due to statistical errors is very small, of the order of  $10^{-9}$ . Work is in progress in order to generalize the methods presented in this work to the case of the triple invariant of Milnor that describes the links formed by three knots.

## ACKNOWLEDGMENTS

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## Appendix A

To compute the nearest point  $\mathbf{x}_{k+1,i}$  of a segment  $\mathbf{l}_{k+1} = \mathbf{x}_{k+1} - \mathbf{x}_k$  from the vertex  $\mathbf{x}_i$ , we pick up on  $\mathbf{l}_{k+1}$  a general point  $\mathbf{X}_{k+1}(\sigma)$  as follows:

$$\mathbf{X}_{k+1}(\sigma) = \mathbf{x}_k + (\mathbf{x}_{k+1} - \mathbf{x}_k)\sigma \quad (\text{A1})$$

with  $\sigma \in [0, 1]$ . The distance between this point and  $\mathbf{x}_i$  is  $\sqrt{(\mathbf{X}_{k+1}(\sigma) - \mathbf{x}_i)^2}$ . If  $\mathbf{X}_{k+1}(\sigma)$  is the nearest point to  $\mathbf{x}_i$ , then it satisfies the condition

$$\frac{d\sqrt{(\mathbf{X}_{k+1}(\sigma) - \mathbf{x}_i)^2}}{d\sigma} = 0 \quad (\text{A2})$$

Inserting Eq. (A1) in (A2) and solving Eq. (A2) with respect to  $\sigma$ , we obtain that the point of  $\mathbf{l}_{k+1}$  at the minimal distance from  $\mathbf{x}_i$  corresponds to the following value of  $\sigma$ :

$$\sigma_{\min} = -\frac{(\mathbf{x}_{k+1} - \mathbf{x}_k) \cdot (\mathbf{x}_k - \mathbf{x}_i)}{(\mathbf{x}_{k+1} - \mathbf{x}_k)^2} \quad (\text{A3})$$

Three cases may occur:

- 1) If  $\sigma_{\min} \geq 1$ , this means that the nearest point occurs on a line having the same direction of  $\mathbf{l}_{k+1}$  at a distance  $\sigma_{\min} \geq 1$  from the point  $\mathbf{x}_k$ . This means that the nearest point to  $\mathbf{x}_i$  on the segment  $\mathbf{l}_{k+1}$  is  $\mathbf{x}_{k+1,i} = \mathbf{x}_{k+1}$  and its distance from  $\mathbf{x}_i$  is  $d_{k+1,i} = |\mathbf{x}_{k+1} - \mathbf{x}_i|$ .



- 2) If  $\sigma_{\min} \leq 0$ , the nearest point occurs on a line having the same direction of  $\mathbf{l}_{k+1}$  at a distance  $-\sigma_{\min}$  from  $\mathbf{x}_k$ . On the segment  $\mathbf{l}_{k+1}$ , the nearest point is in this case the point  $\mathbf{x}_k$ . Its distance from  $\mathbf{x}_i$  is  $d_{k+1,i} = |\mathbf{x}_k - \mathbf{x}_i|$ .
- 3) If  $0 < \sigma_{\min} < 1$ , then  $\mathbf{x}_{k+1,i}$  lies on the segment  $\mathbf{l}_{k+1}$  and  $\mathbf{x}_{k+1,i} = \mathbf{x}_{k+1} + (\mathbf{x}_{k+1} - \mathbf{x}_k)\sigma_{\min}$ . The distance of  $\mathbf{x}_{k+1,i}$  from  $\mathbf{x}_i$  is in this case:

$$d_{k+1,i} = \sqrt{(\mathbf{x}_k - \mathbf{x}_i)^2 - \frac{[(\mathbf{x}_{k+1} - \mathbf{x}_k) \cdot (\mathbf{x}_k - \mathbf{x}_i)]^2}{(\mathbf{x}_{k+1} - \mathbf{x}_k)^2}} \quad (\text{A4})$$

By repeating this procedure for all segments  $\mathbf{l}_{k+1}$  with  $k = 0, \dots, N-1$  and  $k \neq i-1, i$ , we obtain the location of the point of the knot which is not belonging to  $\mathbf{l}_i$  and  $\mathbf{l}_{i+1}$ , and it is the nearest one from  $\mathbf{x}_i$ .

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- <sup>29</sup> We recall that a  $G^1$ -curve is a tangent vector geometrically continuous curve characterized by the fact that the unit tangent vector to the curve is continuous<sup>15</sup>.
- <sup>30</sup> Nonstandard methods like that based on Particle Swarm Optimization proposed in<sup>25</sup> could probably also be applied successfully.
- <sup>31</sup> We do not discuss here the particular case in which  $d_i^{*'} is also equal to zero, which can be easily treated.$